

Problem 5-7 (1-6)

Part 1

If the three given reactions are the only ones occurring, all of the data should be "explained" by the extents of these three reactions. We can calculate ξ_1 , ξ_2 , and ξ_3 from three data points and check to see if these values predict the fourth.



Species	Initial	3Hr.	
A	1	$1 - \xi_1$	$= 0.476$
CHA	0	$\xi_1 - \xi_2 - 2\xi_3$	$= 0.346$
CH	0	ξ_2	$= 0.080$
DCHA	0	ξ_3	$= 0.049$
H ₂	X	$X - 3\xi_1 - \xi_2$	
NH ₃	0	$\xi_2 + \xi_3$	

$$\left. \begin{aligned} \xi_1 &= 0.524 \\ \xi_2 &= 0.080 \\ \xi_3 &= 0.049 \end{aligned} \right\}$$

Use these values to check
CHA

$$0.524 - 0.080 - 2(0.049) \stackrel{?}{=} 0.346 \quad \text{OK}$$

Experimental data is consistent with assumption that three listed reactions are the only ones that occur

Part 2

$$\text{NH}_3 \text{ formed} = \xi_2 + \xi_3 = 0.080 + 0.049 = 0.129$$

moles NH_3 / mole A
charged

Part 3

$$\text{H}_2 \text{ consumed} = 3 \xi_1 + \xi_2 = 3(0.524) + 0.080$$

$$= 1.652 \frac{\text{moles H}_2}{\text{mole A charged}}$$